Thermodynamics of a pseudospin-electron model without correlations

I.V.Stasyuk, A.M.Shvaika, K.V.Tabunshchyk

Institute for Condensed Matter Physics
of the National Academy of Sciences of Ukraine,
1 Svientsitskii Str., 79011 Lviv, Ukraine

Thermodynamics of a pseudospin-electron model without correlations is investigated. The correlation functions, the mean values of pseudospin and particle number, as well as the thermodynamic potential are calculated. The calculation is performed by a diagrammatic method in the mean field approximation. Single-particle Green functions are taken in the Hubbard-I approximation. The numerical research shows that an interaction between the electron and pseudospin subsystems leads in the $\mu = \text{const}$ regime to the possibility of the first order phase transition at the temperature change with the jump of the pseudospin mean value $\langle S^z \rangle$ and reconstruction of the electron spectrum. In the regime $n = \text{const}$, an instability with respect to phase separation in the electron subsystem can take place for certain values of the model parameters.

1. Introduction

The model considering an interaction of electrons with a local anharmonic mode of lattice vibrations has been used in the recent years in the theory of high-temperature superconducting crystals. Particularly, such a property is characteristic of the vibrations of the so-called apex oxygen ions O_{IV} along the c-axis direction of the layered compounds of the $YBa_2Cu_3O_7$-type structure [1, 2, 3]. An important role of the apex oxygen and its anharmonic vibrations in the phase transition into the superconducting state has already been mentioned [4, 5] and a possible connection between the superconductivity and lattice instability of the ferroelectric type in high-T_c superconducting compounds has been discussed [6, 7]. In the case of a local double-well potential, the vibrational degrees of freedom can be presented by pseudospin variables. The Hamiltonian of the derived in this way pseudospin-electron

model has the following form [8]:

$$H = \sum_i H_i + \sum_{ij\sigma} t_{ij} b_{i\sigma}^+ b_{j\sigma}, \tag{1.1}$$

and includes, besides the terms describing electron transfer ($\sim t_{ij}$), the electron correlation (U-term), interaction with the anharmonic mode (g-term), the energy of the tunnelling splitting (Ω-term) and the energy of the anharmonic potential asymmetry (h-term) in the single-site part

$$H_i = U n_{i\uparrow} n_{i\downarrow} + E_0(n_{i\uparrow} + n_{i\downarrow}) + g(n_{i\uparrow} + n_{i\downarrow})S_i^z - \Omega S_i^x - h S_i^z. \tag{1.2}$$

Here, E_0 gives the origin for energies of the electron states at the lattice site ($E_0 = -\mu$).

In this paper, our aim is to obtain expressions for the correlation functions which determine dielectric susceptibility and the mean values of pseudospin and particle number operators, as well as the thermodynamic potential in the case of $\Omega = 0$ and the absence of the Hubbard correlation $U = 0$.

We perform the numerical calculations and investigate the mean values of pseudospin and particle number operators with the change of asymmetry parameter h (T=const) or temperature T (h=const) for the cases of a fixed chemical potential value (regime μ=const) and a constant mean particle number (regime n=const). An analysis of the thermodynamic properties of the pseudospin-electron model in the case of absence of the electron correlation is also made.

2. Hamiltonian and initial relations

We shall write the Hamiltonian of the model and the operators which correspond to physical quantities in the second quantized form using operators of the electron creation (annihilation) at a site with a certain pseudospin orientation

$$a_{i\sigma} = b_{i\sigma}(\frac{1}{2} + S_i^z), \qquad a_{i\sigma}^+ = b_{i\sigma}^+(\frac{1}{2} + S_i^z),$$
$$\tilde{a}_{i\sigma} = b_{i\sigma}(\frac{1}{2} - S_i^z), \qquad \tilde{a}_{i\sigma}^+ = b_{i\sigma}^+(\frac{1}{2} - S_i^z). \tag{2.1}$$

Then, we obtain the following expression for the initial Hamiltonian:

$$\begin{aligned} H &= H_0 + H_{\text{int}} \tag{2.2}\\ &= \sum_i \{\varepsilon(n_{i\uparrow} + n_{i\downarrow}) + \tilde{\varepsilon}(\tilde{n}_{i\uparrow} + \tilde{n}_{i\downarrow}) - hS_i^z\} \\ &+ \sum_{ij\sigma} t_{ij}(a_{i\sigma}^+ a_{j\sigma} + a_{i\sigma}^+ \tilde{a}_{j\sigma} + \tilde{a}_{i\sigma}^+ a_{j\sigma} + \tilde{a}_{i\sigma}^+ \tilde{a}_{j\sigma}), \end{aligned}$$

where

$$\varepsilon = E_0 + g/2, \qquad \tilde{\varepsilon} = E_0 - g/2 \tag{2.3}$$

are energies of the single-site states; H_0 is a single-site (diagonal) term, H_{int} is a hopping term.

The introduced operators satisfy the following commutation rules:

$$\{\tilde{a}_{i\sigma}^+, \tilde{a}_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}(\frac{1}{2} - S_i^z), \qquad \{\tilde{a}_{i\sigma}^+, a_{j\sigma'}\} = 0,$$

$$\{a_{i\sigma}^+, a_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}(\frac{1}{2} + S_i^z), \qquad \{a_{i\sigma}^+, \tilde{a}_{j\sigma'}\} = 0. \tag{2.4}$$

In order to calculate the pseudospin mean values we shall use the standard representation of the statistical operator in the form

$$\mathrm{e}^{-\beta H} = \mathrm{e}^{-\beta H_0}\hat{\sigma}(\beta), \tag{2.5}$$

$$\hat{\sigma}(\beta) = T_\tau \exp\left\{ -\int\limits_0^\beta H_{\mathrm{int}}(\tau)\mathrm{d}\tau \right\}, \tag{2.6}$$

which gives the following expressions for $\langle S_l^z \rangle$:

$$\langle S_l^z \rangle = \frac{1}{\langle \hat{\sigma}(\beta) \rangle_0} \langle S_l^z \hat{\sigma}(\beta) \rangle_0 = \langle S_l^z \hat{\sigma}(\beta) \rangle_0^{\mathrm{c}}. \tag{2.7}$$

Here, the operators are given in the interaction representation

$$A(\tau) = \mathrm{e}^{\tau H_0} A \mathrm{e}^{-\tau H_0}, \tag{2.8}$$

the averaging $\langle \ldots \rangle_0$ is performed over statistical distribution with the Hamiltonian H_0, and the symbol $\langle \ldots \rangle_0^{\mathrm{c}}$ denotes separation of connected diagrams.

3. Perturbation theory for pseudospin mean values and a diagram technique

Expansion of the exponent in (2.6) in powers of H_{int} (2.2) leads, after substitution in equation (2.7), to an expression that has the form of the sum of infinite series with terms containing the averages of the T-products of the electron creation (annihilation) operators (2.1). The evaluation of such averages can be made using the Wick theorem.

In our case this theorem has some differences from the standard formulation. Namely, each pairing of operators (2.1) contains operator factors, i.e.

$$\overset{\frown}{a_i(\tau')a_o^+(\tau)} = \breve{g}(\tau' - \tau)\delta_{io}P_i^+, \quad \overset{\frown}{\tilde{a}_i(\tau')\tilde{a}_o^+(\tau)} = \tilde{g}(\tau' - \tau)\delta_{io}P_i^-, \tag{3.1}$$

$$\overset{\frown}{a_o^+(\tau)a_i(\tau')} = -\breve{g}(\tau' - \tau)\delta_{io}P_i^+, \quad \overset{\frown}{\tilde{a}_o^+(\tau)\tilde{a}_i(\tau')} = -\tilde{g}(\tau' - \tau)\delta_{io}P_i^-.$$

Finally, this gives the possibility to express the result in terms of the products of nonperturbed Green functions

$$\breve{g}_{io}(\tau - \tau') = \frac{\langle T_\tau a_i(\tau)a_o^+(\tau') \rangle_0}{\langle \{a_i a_o^+\} \rangle_0} = \mathrm{e}^{\varepsilon(\tau'-\tau)}\delta_{oi}\begin{cases} (1 + \mathrm{e}^{-\beta\varepsilon})^{-1} & , \tau > \tau', \\ -(1 + \mathrm{e}^{\beta\varepsilon})^{-1} & , \tau' > \tau, \end{cases} \tag{3.2}$$

$$\tilde{g}_{io}(\tau - \tau') = \frac{\langle T_\tau \tilde{a}_i(\tau)\tilde{a}_o^+(\tau')\rangle_0}{\langle \{\tilde{a}_i \tilde{a}_o^+\}\rangle_0} = \mathrm{e}^{\tilde{\varepsilon}(\tau'-\tau)}\delta_{oi} \left\{ \begin{array}{ll} (1 + \mathrm{e}^{-\beta\tilde{\varepsilon}})^{-1} & , \tau > \tau', \\ -(1 + \mathrm{e}^{\beta\tilde{\varepsilon}})^{-1} & , \tau' > \tau, \end{array} \right.$$

$$\tilde{g}_{io}(\tau - \tau') = \tilde{g}(\tau - \tau')\delta_{io}, \qquad \breve{g}_{io}(\tau - \tau') = \breve{g}(\tau - \tau')\delta_{io},$$

and averages of a certain number of the projection operators

$$P_i^+ = \frac{1}{2} + S_i^z, \qquad P_i^- = \frac{1}{2} - S_i^z. \tag{3.3}$$

Let us demonstrate this procedure for one of the terms which appear in the fourth order of the perturbation theory for $\langle S_l^z \rangle$:

$$\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3 \int_0^\beta d\tau_4 \sum_{iji_1j_1} \sum_{i_2j_2i_3j_3} t_{ij}t_{i_1j_1}t_{i_2j_2}t_{i_3j_3} \tag{3.4}$$

$$\times \langle T_\tau S_l^z a_i^+(\tau_1)a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{j_1}(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)a_{j_3}(\tau_4)\rangle_0.$$

The stepwise pairing of a certain operator with the other ones gives the possibility to reduce expression (3.4) to the sum of the averages of a smaller number of operators

$$\langle T_\tau S_l^z a_i^+(\tau_1)a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{j_1}(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)a_{j_3}(\tau_4)\rangle_0$$

$$= \langle T_\tau S_l^z \overbrace{a_i^+(\tau_1)}a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{j_1}(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)\overbrace{a_{j_3}(\tau_4)}\rangle_0$$

$$+ \langle T_\tau S_l^z \overbrace{a_i^+(\tau_1)}a_j(\tau_1)\overbrace{\tilde{a}_{i_1}^+(\tau_2)}a_{j_1}(\tau_2)\ a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)a_{j_3}(\tau_4)\rangle_0$$

$$= -\breve{g}_{ij_3}(\tau_1 - \tau_4)\langle T_\tau S_l^z P_{j_3}^+ a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{j_1}(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)\rangle_0 \tag{3.5}$$

$$- \breve{g}_{ij_1}(\tau_1 - \tau_2)\langle T_\tau S_l^z P_{j_1}^+ a_j(\tau_1)\tilde{a}_{i_1}^+(\tau_2)a_{i_2}^+(\tau_3)\tilde{a}_{j_2}(\tau_3)a_{i_3}^+(\tau_4)a_{j_2}(\tau_3)\rangle_0.$$

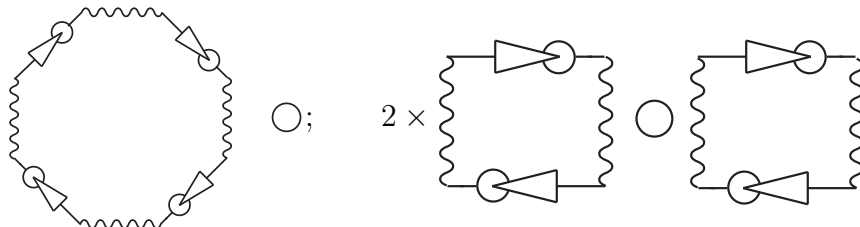The successive application of the pairing procedure for (3.5) leads, finally, to

$$-\breve{g}_{ij_1}(\tau_1-\tau_2)\tilde{g}_{i_1j_2}(\tau_2-\tau_3)\breve{g}_{i_3j}(\tau_4-\tau_1)\breve{g}_{i_2j_1}(\tau_3-\tau_2)\langle T_\tau S_l^z P_j^+ P_{j_1}^+ P_{j_2}^- P_{j_3}^+\rangle_0$$
$$-\breve{g}_{ij_3}(\tau_1-\tau_4)\tilde{g}_{i_1j_2}(\tau_2-\tau_3)\breve{g}_{i_2j}(\tau_3-\tau_1)\breve{g}_{i_3j_1}(\tau_4-\tau_2)\langle T_\tau S_l^z P_j^+ P_{j_1}^+ P_{j_2}^- P_{j_3}^+\rangle_0 \tag{3.6}$$
$$+\breve{g}_{ij_3}(\tau_1-\tau_4)\tilde{g}_{i_1j_2}(\tau_2-\tau_3)\breve{g}_{i_2j_1}(\tau_3-\tau_2)\breve{g}_{i_3j}(\tau_4-\tau_1)\langle T_\tau S_l^z P_j^+ P_{j_1}^+ P_{j_2}^- P_{j_3}^+\rangle_0.$$
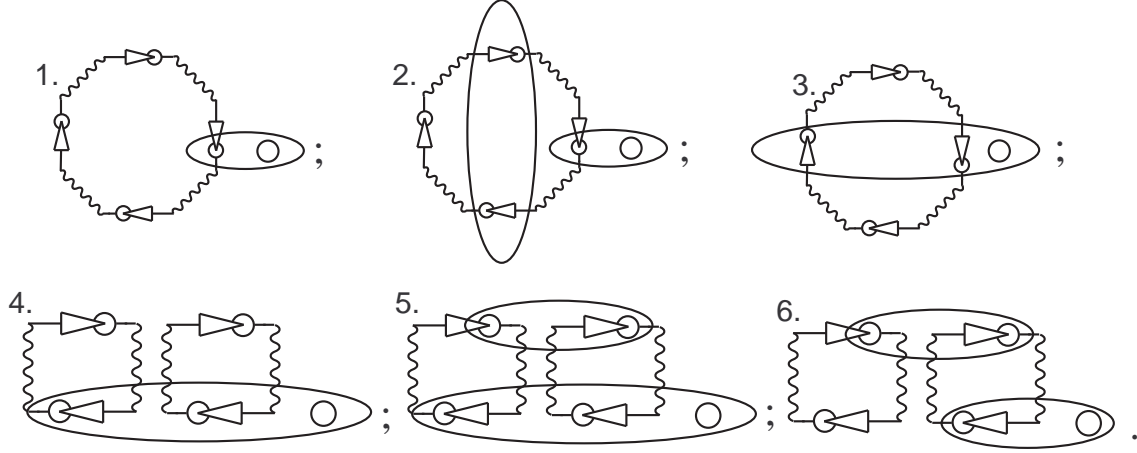
We introduce the diagrammatic notations

$$\bigcirc - S_l^z; \qquad 1\!\sim\!\sim\!\sim\!\sim\!1' - t_{11'};$$
$$1\!-\!\!\rhd\!\!-\!\!1' - (\breve{g}_{11'}P_1^+ + \tilde{g}_{11'}P_1^-)$$

and diagrams

which correspond to expression (3.6).

Expansion of (3.6) in semi-invariants leads to multiplication of diagrams (semi-invariants are represented by ovals surrounding the corresponding vertices with diagonal operators and contain the δ-symbol on site indexes). For example,

We shall omit diagrams of types 2, 3, 5, i.e. the types including semi-invariants of a higher than the first order in the loop (this means that chain fragments form single-electron Green functions in the Hubbard-I approximation) and also connection of two loops by more than one semi-invariant (this approximation means that a self-consistent field is taken into account in the zero approximation).

Let us proceed to the momentum-frequency representation in the expressions for the Green functions determined on a finite interval $0<\tau<\beta$ when they can be expanded in the Fourier series with discrete frequencies

$$\breve{g}(\tau) = \frac{1}{\beta} \sum_n e^{i\omega_n\tau} \breve{g}(\omega_n), \qquad \tilde{g}(\tau) = \frac{1}{\beta} \sum_n e^{i\omega_n\tau} \tilde{g}(\omega_n), \qquad (3.7)$$

$$\breve{g}(\omega_n) = -\frac{1}{i\omega_n - \varepsilon}, \qquad \tilde{g}(\omega_n) = -\frac{1}{i\omega_n - \tilde{\varepsilon}}, \qquad \omega_n = \frac{2n+1}{\beta}\pi.$$

The characteristic feature of the already presented diagrams and the diagrams corresponding to other orders of the perturbation theory is the presence of chain fragments. The simplest series of chain diagrams is

where

$$\longrightarrow\!\!\triangleright\!\!\bullet\!\!\longrightarrow = g(\omega_n) = \frac{\langle P^+\rangle}{i\omega_n - \varepsilon} + \frac{\langle P^-\rangle}{i\omega_n - \tilde{\varepsilon}} \qquad (3.9)$$
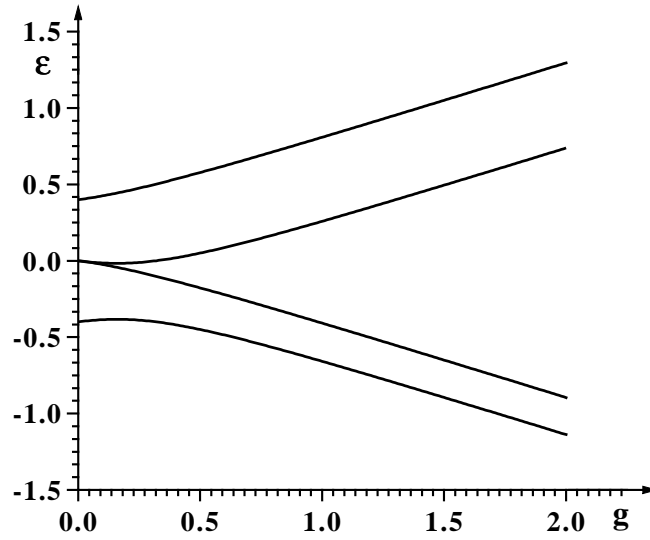
and corresponds to the Hubbard-I approximation for a single-electron Green function. The expression

$$\Longrightarrow\!\!\triangleright\!\!= = G_{\boldsymbol{k}}(\omega_n) = \frac{1}{g^{-1}(\omega_n) - t_{\boldsymbol{k}}} \qquad (3.10)$$

in the momentum-frequency representation corresponds to the sum of graphs (3.8). The poles of function $G_{\boldsymbol{k}}(\omega_n)$ determine the spectrum of the single-electron excitations

$$\varepsilon_{\mathrm{I,II}}(t_{\boldsymbol{k}}) = \frac{1}{2}(2E_0 + t_{\boldsymbol{k}}) \pm \frac{1}{2}\sqrt{g^2 + 4t_{\boldsymbol{k}}\langle S^z \rangle g + t_{\boldsymbol{k}}^2}. \tag{3.11}$$

Behaviour of the electron bands as a function of the coupling constant is presented in figure 1. One can see that there always exists a gap in the spectrum. The widths of subbands depends on the mean value of the pseudospin and in the case of strong coupling ($g \gg W$) the subbands' halfwidth is equal to $W(\frac{1}{2} \pm \langle S^z \rangle)$ (W is the halfwidth of the initial electron band).

Figure 1. Electron bands boundaries ($W = 0.4$, $\langle S^z \rangle = 0.2$).

Let us now return to the problem of summation of the diagram series for the mean value $\langle S_l^z \rangle$ taking into account the above mentioned arguments. The diagram series has the form

$$\tag{3.12}$$

The analytical expressions for the loop has the following form

$$\begin{aligned}
&= \frac{2}{N}\sum_{n,\boldsymbol{k}} \frac{t_{\boldsymbol{k}}^2}{g^{-1}(\omega_n) - t_{\boldsymbol{k}}}\left(\frac{P_i^+}{\mathrm{i}\omega_n - \varepsilon} + \frac{P_i^-}{\mathrm{i}\omega_n - \tilde{\varepsilon}}\right) \\
&= \beta(\alpha_1 P_i^+ + \alpha_2 P_i^-),
\end{aligned} \tag{3.13}$$

where we used the notations

$$\alpha_1 = \frac{2}{N\beta} \sum_{n,\boldsymbol{k}} \frac{t_{\boldsymbol{k}}^2}{(g^{-1}(\omega_n) - t_{\boldsymbol{k}})} \frac{1}{(\mathrm{i}\omega_n - \varepsilon)}, \quad \alpha_2 = \frac{2}{N\beta} \sum_{n,\boldsymbol{k}} \frac{t_{\boldsymbol{k}}^2}{(g^{-1}(\omega_n) - t_{\boldsymbol{k}})} \frac{1}{(\mathrm{i}\omega_n - \tilde{\varepsilon})}.$$

Using decomposition into simple fractions and summation over frequency we obtain

$$\alpha_1 = \frac{2}{N} \sum_{\boldsymbol{k}} t_{\boldsymbol{k}} \Big[A_1 n(\varepsilon_\mathrm{I}(t_{\boldsymbol{k}})) + B_1 n(\varepsilon_\mathrm{II}(t_{\boldsymbol{k}})) \Big], \quad \alpha_2 = \frac{2}{N} \sum_{\boldsymbol{k}} t_{\boldsymbol{k}} \Big[A_2 n(\varepsilon_\mathrm{I}(t_{\boldsymbol{k}})) + B_2 n(\varepsilon_\mathrm{II}(t_{\boldsymbol{k}})) \Big],$$

where

$$A_1 = \frac{\varepsilon_\mathrm{I}(t_{\boldsymbol{k}}) - \tilde{\varepsilon}}{\varepsilon_\mathrm{I}(t_{\boldsymbol{k}}) - \varepsilon_\mathrm{II}(t_{\boldsymbol{k}})}, \qquad B_1 = \frac{\varepsilon_\mathrm{II}(t_{\boldsymbol{k}}) - \tilde{\varepsilon}}{\varepsilon_\mathrm{II}(t_{\boldsymbol{k}}) - \varepsilon_\mathrm{I}(t_{\boldsymbol{k}})},$$

$$A_2 = \frac{\varepsilon_\mathrm{I}(t_{\boldsymbol{k}}) - \varepsilon}{\varepsilon_\mathrm{I}(t_{\boldsymbol{k}}) - \varepsilon_\mathrm{II}(t_{\boldsymbol{k}})}, \qquad B_2 = \frac{\varepsilon_\mathrm{II}(t_{\boldsymbol{k}}) - \varepsilon}{\varepsilon_\mathrm{II}(t_{\boldsymbol{k}}) - \varepsilon_\mathrm{I}(t_{\boldsymbol{k}})},$$

and $n(\varepsilon) = \dfrac{1}{1 + \mathrm{e}^{\beta\varepsilon}}$ is a Fermi distribution.

The equation for $\langle S_l^z \rangle$ can be presented in the form

$$\begin{aligned}
\langle S_l^z \rangle &= \langle S_l^z \rangle_0 - \langle S_l^z \beta(\alpha_1 P_l^+ + \alpha_2 P_l^-) \rangle_0^\mathrm{c} \\
&\quad + \frac{1}{2!} \langle S_l^z \beta^2 (\alpha_1 P_l^+ + \alpha_2 P_l^-)^2 \rangle_0^\mathrm{c} - \ldots = \langle S_l^z \mathrm{e}^{-\beta(\alpha_1 P_l^+ + \alpha_2 P_l^-)} \rangle_0^\mathrm{c}.
\end{aligned} \tag{3.14}$$

Let us introduce

$$H_\mathrm{MF} = \sum_i H_i^\mathrm{MF},$$

where

$$H_i^\mathrm{MF} = H_{i\,0} + \alpha_1 P_i^+ + \alpha_2 P_i^-.$$

Then, the analytical equation for $\langle S_l^z \rangle$ can be expressed in the form

$$\begin{aligned}
\langle S_l^z \rangle = \langle S_l^z \rangle_\mathrm{MF} &= \frac{\mathrm{Sp}(S_l^z \mathrm{e}^{-\beta H_\mathrm{MF}})}{\mathrm{Sp}(\mathrm{e}^{-\beta H_\mathrm{MF}})} \\
&= \frac{1}{2} \tanh \left\{ \frac{\beta}{2}(h + \alpha_2 - \alpha_1) + \ln \frac{1 + \mathrm{e}^{-\beta\varepsilon}}{1 + \mathrm{e}^{-\beta\tilde{\varepsilon}}} \right\}.
\end{aligned} \tag{3.15}$$

The difference $\alpha_2 - \alpha_1$ corresponds to an internal effective self-consistent field acting on the pseudospin

$$\alpha_2 - \alpha_1 = \frac{2}{N} \sum_{\boldsymbol{k}} t_{\boldsymbol{k}} \frac{\varepsilon - \tilde{\varepsilon}}{\varepsilon_\mathrm{I}(t_{\boldsymbol{k}}) - \varepsilon_\mathrm{II}(t_{\boldsymbol{k}})} \Big[n(\varepsilon_\mathrm{II}(t_{\boldsymbol{k}})) - n(\varepsilon_\mathrm{I}(t_{\boldsymbol{k}})) \Big]. \tag{3.16}$$

4. The mean value of the particle number

The diagram series for the mean value $\langle n_i \rangle$ (using the perturbation theory, the Wick theorem and expansion in semi-invariants) can be presented in the form

where

$$P^\alpha = (P^+; P^-), \qquad \varepsilon_\alpha = (\varepsilon; \tilde{\varepsilon})$$

and the last term appears due to the pairing of the electron creation (annihilation) operators with the operator of the particle number.

An analytical expression for (4.1) can be obtained starting from formulae (3.9), (3.10):

$$\langle n_i \rangle = \langle n_i \rangle_{\mathrm{MF}} + \frac{2}{N\beta} \sum_{n,\boldsymbol{k},\alpha} \frac{t_{\boldsymbol{k}}^2}{(g^{-1}(\omega_n) - t_{\boldsymbol{k}})} \frac{\langle P^\alpha \rangle}{(\mathrm{i}\omega_n - \varepsilon^\alpha)^2}. \tag{4.2}$$

Using decomposition into simple fractions and summation over frequency we can present the mean value $\langle n_i \rangle$ in the form:

$$\langle n_i \rangle = \frac{2}{N} \sum_{\boldsymbol{k}} \left[n(\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})) + n(\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})) \right] - 2\langle P^+ \rangle n(\tilde{\varepsilon}) - 2\langle P^- \rangle n(\varepsilon). \tag{4.3}$$

5. Thermodynamic potential

In order to calculate the thermodynamic potential let us introduce parameter $\lambda \in [0, 1]$ in the initial Hamiltonian

$$H_\lambda = H_0 + \lambda H_{\mathrm{int}}, \tag{5.1}$$

such that $H \to H_0$ for $\lambda = 0$ and $H \to H_0 + H_{\mathrm{int}}$ for $\lambda = 1$.

Hence,

$$Z_\lambda = \mathrm{Sp}(\mathrm{e}^{-\beta H_\lambda}) = \mathrm{Sp}(\mathrm{e}^{-\beta H_0} \hat{\sigma}_\lambda(\beta)) = Z_0 \langle \hat{\sigma}_\lambda(\beta) \rangle_0,$$

where

$$\hat{\sigma}_\lambda(\beta) = T_\tau \exp \left\{ -\lambda \int_0^\beta H_{\mathrm{int}}(\tau) \mathrm{d}\tau \right\},$$

and

$$\Omega_\lambda = -\frac{1}{\beta}\ln Z_0 - \frac{1}{\beta}\ln\langle\hat{\sigma}_\lambda(\beta)\rangle_0, \tag{5.2}$$

$$\Delta\Omega_\lambda = \Omega_\lambda - \Omega_0 = -\frac{1}{\beta}\ln\langle\hat{\sigma}_\lambda(\beta)\rangle_0.$$

Here Ω_0 is a thermodynamic potential calculated with the single-site (diagonal) part of the initial Hamiltonian.

Therefore,

$$\Delta\Omega = \int_0^1 d\lambda\left(\frac{d\Omega_\lambda}{d\lambda}\right). \tag{5.3}$$

For value $d\Omega_\lambda/d\lambda$, we can immediately write the diagram series in the next form:

$$\beta\frac{d\Omega_\lambda}{d\lambda} = \ldots \tag{5.4}$$

where $ - \lambda t$, and also

Expression (5.3) can be presented in the form (using the diagram series (5.4)):

$$\Delta\Omega = \frac{2}{N\beta}\sum_{n,\boldsymbol{k}}\int_0^1 \lambda t_{\boldsymbol{k}}^2 g_\lambda^2(\omega_n)\frac{1}{1-\lambda t_{\boldsymbol{k}}g_\lambda(\omega_n)}d\lambda$$

$$= -\frac{2}{N\beta}\sum_{n,\boldsymbol{k}}\ln(1-t_{\boldsymbol{k}}g(\omega_n)) - \frac{2}{N\beta}\sum_{n,\boldsymbol{k}}\int_0^1 \frac{\lambda t_{\boldsymbol{k}}\frac{dg_\lambda(\omega_n)}{d\lambda}}{1-\lambda t_{\boldsymbol{k}}g_\lambda(\omega_n)}d\lambda. \tag{5.5}$$

The first term in expression (5.5) may be written in a diagram form as

$$(5.6)$$

Series (5.6) describes an electron gas whose energy spectrum is defined by the total pseudospin field. This series is in conformity with the so-called one-loop approximation.

The second term in expression (5.5) can be integrated to the following diagram series

$$(5.7)$$

and appears due to the presence of a pseudospin subsystem.

Finally, the diagram series for $\beta \Delta\Omega$ can be written as a sum of expressions (5.6) and (5.7), and the corresponding analytical expression is the following:

$$
\Delta\Omega = -\frac{2}{N\beta} \sum_{\boldsymbol{k}} \ln \frac{(\cosh \frac{\beta}{2}\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}))(\cosh \frac{\beta}{2}\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}}))}{(\cosh \frac{\beta}{2}\varepsilon)(\cosh \frac{\beta}{2}\tilde{\varepsilon})}
$$
$$
-\frac{1}{\beta} \ln \cosh \left\{ \frac{\beta}{2}(h + \alpha_2 - \alpha_1) + \ln \frac{1 + \mathrm{e}^{-\beta\varepsilon}}{1 + \mathrm{e}^{-\beta\tilde{\varepsilon}}} \right\}
$$
$$
+\frac{1}{\beta} \ln \cosh \left\{ \frac{\beta}{2}h + \ln \frac{1 + \mathrm{e}^{-\beta\varepsilon}}{1 + \mathrm{e}^{-\beta\tilde{\varepsilon}}} \right\} + \langle S^z \rangle (\alpha_2 - \alpha_1). \qquad (5.8)
$$

Here, decomposition in simple fractions and summation over frequency were done.

Then, since the thermodynamic potential is a function of the argument $\langle S^z \rangle$, let us check the consistency of approximations made for $\langle S^z \rangle$, $\langle n \rangle$ and thermodynamic potential Ω. For this purpose let us derive the mean values $\langle S^z \rangle$ and $\langle n \rangle$ from the expression for the grand thermodynamic potential

$$
\frac{\mathrm{d}\Omega}{\mathrm{d}(-\mu)} = \frac{2}{N} \sum_{\boldsymbol{k}} \left[n(\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})) + n(\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})) \right] - 2\langle P^+ \rangle n(\tilde{\varepsilon}) - 2\langle P^- \rangle n(\varepsilon),
$$

$$
\frac{\mathrm{d}\Omega}{\mathrm{d}(-h)} = \frac{1}{2} \tanh \left\{ \frac{\beta}{2}(h + \alpha_2 - \alpha_1) + \ln \frac{1 + \mathrm{e}^{-\beta\varepsilon}}{1 + \mathrm{e}^{-\beta\tilde{\varepsilon}}} \right\}.
$$

We thus obtain

$$\frac{\mathrm{d}\Omega}{\mathrm{d}(-\mu)} = \langle n \rangle, \qquad\qquad \frac{\mathrm{d}\Omega}{\mathrm{d}(-h)} = \langle S^z \rangle.$$

Therefore, the calculation of the mean values of the pseudospin and particle number operators as well as the thermodynamic potential is performed in the same approximation which corresponds to the mean field one.

6. Pseudospin, electron and mixed correlators

In this section our aim is to calculate the correlators

$$
\begin{aligned}
K_{lm}^{ss}(\tau - \tau') &= \langle T \tilde{S}_l^z(\tau) \tilde{S}_m^z(\tau') \rangle^{\mathrm{c}}, \\
K_{lm}^{sn}(\tau - \tau') &= \langle T \tilde{S}_l^z(\tau) \tilde{n}_m(\tau') \rangle^{\mathrm{c}}, \\
K_{lm}^{nn}(\tau - \tau') &= \langle T \tilde{n}_l(\tau) \tilde{n}_m(\tau') \rangle^{\mathrm{c}},
\end{aligned}
$$

constructed of the operators given in the Heisenberg representation with an imaginary time argument.

Let us present a diagram series for the correlation function (in the momentum-frequency representation) within a self-consistent scheme in the framework of the generalized random phase approximation (GRPA) (which was applied in [9, 10] where the magnetic susceptibility of the ordinary Hubbard model and $t - J$ model was considered). In our case (the absence of the Hubbard correlation) this approximation is reduced, because the so-called ladder diagrams [11] with antiparallel lines disappear.

We would like to remind that we have omitted diagrams including semi-invariants of a higher than the first order in the loop and also connection of two loops by more than one semi-invariant.

$$\langle S^z S^z \rangle_{\boldsymbol{q}} = \quad \cdots \qquad\qquad (6.1)$$

where we define

$$= \Gamma^\alpha(\boldsymbol{k}, \omega_n);$$

$$P^\alpha = (P^+, P^-); \quad \alpha = (0,1); \quad \varepsilon^\alpha = (\varepsilon, \tilde{\varepsilon}); \quad \textcircled{\alpha} = P^\alpha; \quad \bigcirc = S^z \quad.$$

Here, the first term in equation (6.1) takes into account a direct influence of the internal effective self-consistent field on pseudospins and is given by

$$\tag{6.2}$$

Series (6.2) means a second-order semi-invariant renormalized due to the "single-tail" parts, and is thus calculated by H_{MF}.

The second term in equation (6.1) describes an interaction between pseudospins which is mediated by electrons (the energy of the electron spectrum is defined by the total pseudospin field).

We introduce the shortened notations

$$\tag{6.3}$$

Solution of equation (6.1) can be written in the analytical form

$$\langle S^z S^z \rangle_{\boldsymbol{q}} = \frac{1/4 - \langle S^z \rangle^2}{1 + \sum\limits_{\alpha,\beta} (-1)^{\alpha+\beta} \boxed{\Pi}_{\boldsymbol{q}}^{\alpha,\beta} (\frac{1}{4} - \langle S^z \rangle^2)}, \tag{6.4}$$

where

$$\boxed{\Pi}_{\boldsymbol{q}}^{\alpha,\beta} = \frac{2}{N} \sum_{n,\boldsymbol{k}} t_{\boldsymbol{k}} t_{\boldsymbol{k}+\boldsymbol{q}} \Gamma^{\alpha}(\boldsymbol{k}, \omega_n) \Gamma^{\beta}(\boldsymbol{k}+\boldsymbol{q}, \omega_n), \tag{6.5}$$

$$\Gamma^{\alpha}(\boldsymbol{k}, \omega_n) = \frac{1}{(\mathrm{i}\omega_n - \varepsilon^{\alpha})} \frac{1}{(1 - t_{\boldsymbol{k}} g(\omega_n))}. \tag{6.6}$$

Decomposition of function $\Gamma^{\alpha}(\boldsymbol{k}, \omega_n)$ into simple fractions and the subsequent evaluation of the sum over frequency leads to the next expression:

$$\sum_{\alpha,\beta} (-1)^{\alpha+\beta} \boxed{\Pi}_{\boldsymbol{q}}^{\alpha,\beta} = \frac{2\beta}{N} \sum_{\boldsymbol{k}} \frac{t_{\boldsymbol{k}} t_{\boldsymbol{k}+\boldsymbol{q}} (\varepsilon - \tilde{\varepsilon})^2}{[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})][\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}$$

$$\times \left\{ \frac{n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}{\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}})} + \frac{n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}{\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})} \right.$$

$$\left. - \frac{n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}{\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})} - \frac{n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}{\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}})} \right\}. \tag{6.7}$$

After substitution (6.7) in equation (6.4) we finally obtain an expression for $\langle S^z S^z \rangle_{\boldsymbol{q}}$.

This formula for the uniform case ($\boldsymbol{q} = 0$) can be rewritten as

$$\langle S^z S^z \rangle_{\boldsymbol{q}=0} = (1/4 - \langle S^z \rangle^2) \tag{6.8}$$
$$\times \left\{ 1 - \left(\frac{4\beta}{N} \sum_{\boldsymbol{k}} t_{\boldsymbol{k}}^2 \frac{(\varepsilon - \tilde{\varepsilon})^2}{[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})]^3} \{ n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})] \} \right. \right.$$
$$\left. \left. + \frac{\beta^2}{2N} \sum_{\boldsymbol{k}} \frac{t_{\boldsymbol{k}}^2(\varepsilon - \tilde{\varepsilon})^2}{[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})]^2} \left\{ \frac{1}{\cosh^2 \frac{\beta \varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})}{2}} + \frac{1}{\cosh^2 \frac{\beta \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})}{2}} \right\} \right) \left(\frac{1}{4} - \langle S^z \rangle^2 \right) \right\}^{-1}.$$

Expression (6.8) can be obtained from the derivative $\mathrm{d}\langle S^z \rangle / \mathrm{d}(\beta h)$. This means that the mean values of the pseudospin and pseudospin correlators are derived in the same approximation.

For a mixed correlator the diagram series has the form

$$\tag{6.9}$$

where

$$\tag{6.10}$$

$$\tag{6.11}$$

$$= P^\alpha \Gamma^\alpha(\boldsymbol{k}, \omega_n).$$

Solution of equation (6.10) can be written in the analytical form

$$I = 2(n(\varepsilon) - n(\tilde{\varepsilon}))\langle S^z S^z \rangle_{\boldsymbol{q}}. \tag{6.12}$$

Here we start from formula (6.4) and from the next relation:

$$\frac{\langle S^z n \rangle_{\mathrm{MF}} - \langle S^z \rangle \langle n \rangle}{\frac{1}{4} - \langle S^z \rangle^2} = 2(n(\varepsilon) - n(\tilde{\varepsilon})). \tag{6.13}$$

The second term in diagram series (6.9) can be presented as

$$
\begin{aligned}
II = {} & \frac{2}{N}\langle S^z S^z\rangle_{\boldsymbol{q}} \sum_{\boldsymbol{k}} \frac{t_{\boldsymbol{k}}(\varepsilon - \tilde{\varepsilon})}{\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})} \\
& \times \Bigg[\frac{n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}{\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}})} + \frac{n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}{\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})} \\
& - \frac{n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}{\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}+\boldsymbol{q}})} - \frac{n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})] - n[\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})]}{\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}+\boldsymbol{q}})} \Bigg] .
\end{aligned}
\tag{6.14}
$$

Let us introduce the shortened notations for expression (6.14)

$$
II = \langle S^z S^z\rangle_{\boldsymbol{q}}[\oplus]_{\boldsymbol{q}}.
\tag{6.15}
$$

In this way we obtain

$$
\langle S^z n\rangle_{\boldsymbol{q}} = 2\Big[n(\varepsilon) - n(\tilde{\varepsilon})\Big]\langle S^z S^z\rangle_{\boldsymbol{q}} + \langle S^z S^z\rangle_{\boldsymbol{q}}[\oplus]_{\boldsymbol{q}}.
\tag{6.16}
$$

From our diagram series we can see: correlators containing the pseudospin variable S^z are different from zero only in a static case. This is due to the fact that operator S^z commutes with the Hamiltonian, being an integral of motion.

For an electron correlator our diagram series has the form:

and only the last term is not equal to zero for non-zero frequencies. Let us consider series (6.17) term by term.

The first term in series (6.17) may be written as

After simple transformation we can obtain the next relation:

$$
\langle nn\rangle_{\mathrm{MF}} - \langle n\rangle^2 - \frac{1}{2}\left(\frac{\langle P^+\rangle}{\cosh^2 \frac{\beta\varepsilon}{2}} + \frac{\langle P^-\rangle}{\cosh^2 \frac{\beta\tilde{\varepsilon}}{2}} \right) = \frac{(\langle nS^z\rangle_{\mathrm{MF}} - \langle n\rangle\langle S^z\rangle)^2}{\langle P^+\rangle\langle P^-\rangle}.
\tag{6.19}
$$

This relation makes it possible to write immediately a simple analytical expression for series (6.18)

$$
I = \left\{ [2(n(\varepsilon) - n(\tilde{\varepsilon}))]^2\langle S^z S^z\rangle_{\boldsymbol{q}} + \frac{1}{2}\left(\frac{\langle P^+\rangle}{\cosh^2 \frac{\beta\varepsilon}{2}} + \frac{\langle P^-\rangle}{\cosh^2 \frac{\beta\tilde{\varepsilon}}{2}} \right) \right\}\delta(\omega).
\tag{6.20}
$$

Analytical expressions for the II-term can be obtained starting from formulae (6.11)–(6.15)

$$II = \left\{ 2[n(\varepsilon) - n(\tilde{\varepsilon})]\langle S^z S^z\rangle_{\boldsymbol{q}}[\oplus]_{\boldsymbol{q}} \right\}\delta(\omega). \tag{6.21}$$

Using expression (6.16) we can unite (6.21) and (6.20)

$$I + II = \left\{ 2(n(\varepsilon) - n(\tilde{\varepsilon}))\langle S^z n\rangle_{\boldsymbol{q}} + \frac{1}{2}\left(\frac{\langle P^+\rangle}{\cosh^2 \frac{\beta\varepsilon}{2}} + \frac{\langle P^-\rangle}{\cosh^2 \frac{\beta\tilde{\varepsilon}}{2}} \right) \right\}\delta(\omega). \tag{6.22}$$

The diagram series for the fourth term in (6.17) has the form

and can be written as

$$IV = \quad = [\oplus]_{\boldsymbol{q}}\langle S^z S^z\rangle_{\boldsymbol{q}}[\oplus]_{\boldsymbol{q}}\delta(\omega). \tag{6.23}$$

Using formula (6.16) once more we unite the III-term and the IV-term

$$III + IV = \langle n S^z\rangle_{\boldsymbol{q}}[\oplus]_{\boldsymbol{q}}\delta(\omega). \tag{6.24}$$

The last term can be presented in the form

$$\tag{6.25}$$

Let us write down the final formula for an electron correlator for the uniform ($\boldsymbol{q} = 0$) and static ($\omega = 0$) case

$$\langle nn\rangle = 2(n(\varepsilon) - n(\tilde{\varepsilon}))\langle S^z n\rangle_{\boldsymbol{q}=0} + \frac{1}{2}\left(\frac{\langle P^+\rangle}{\cosh^2 \frac{\beta\varepsilon}{2}} + \frac{\langle P^-\rangle}{\cosh^2 \frac{\beta\tilde{\varepsilon}}{2}} \right) \tag{6.26}$$

$$+\frac{\beta}{2N}\sum_{\boldsymbol{k}} \frac{t_{\boldsymbol{k}}(\varepsilon - \tilde{\varepsilon})}{\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}}) - \varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})}\left\{ \frac{1}{\cosh^2 \frac{\beta\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})}{2}} - \frac{1}{\cosh^2 \frac{\beta\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})}{2}} \right\}\langle S^z n\rangle_{\boldsymbol{q}=0}$$

$$+\frac{1}{2N}\sum_{\boldsymbol{k}}\left\{ \frac{1}{\cosh^2 \frac{\beta\varepsilon_{\mathrm{II}}(t_{\boldsymbol{k}})}{2}} + \frac{1}{\cosh^2 \frac{\beta\varepsilon_{\mathrm{I}}(t_{\boldsymbol{k}})}{2}} \right\} - \frac{1}{2}\left\{ \frac{1}{\cosh^2 \frac{\beta\varepsilon}{2}} + \frac{1}{\cosh^2 \frac{\beta\tilde{\varepsilon}}{2}} \right\}.$$

The same result can be obtained from the derivative $\mathrm{d}\langle n\rangle/(\mathrm{d}\beta\mu)$. Thus, all our quantities: the mean values of the pseudospin and particle number operators, the thermodynamic potential as well as correlation functions are derived within the framework of one approximation which corresponds to the mean field approximation.
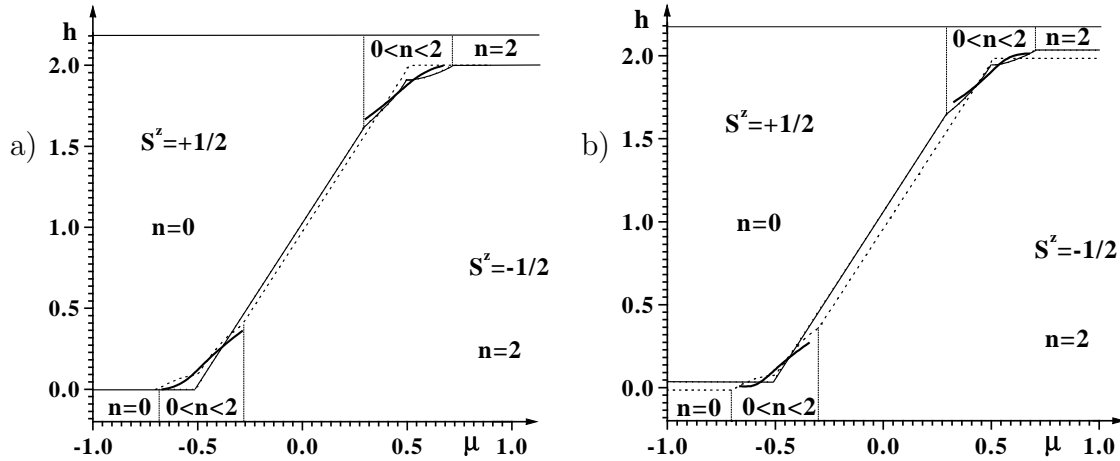
7. Numerical research in the $\mu = $ const regime

In the investigation of equilibrium conditions we shall separate two regimes: μ=const and n=const. For the first regime the equilibrium is defined by the minimum of the thermodynamic potential: $\left(\frac{\partial\Omega}{\partial\langle S^z\rangle}\right)_{T,\mu,h} = 0$.

The μ=const regime corresponds to the case when charge redistribution between the conducting sheets CuO_2 and other structural elements (charge reservoir, e.g., nonstoichiometric in oxygen CuO chains in YBaCuO-type structures) is allowed.

The dependencies of the order parameter $\langle S^z\rangle$ on field h and temperature T at the constant value of the chemical potential are determined by equation (3.15). All the integrals in (3.15) can be calculated analytically at zero temperature (below, all the calculations will be performed for the rectangular density of states, but we would like to note that the similar behaviour can be obtained in the case of the semi-elliptic density of states).

We shall present all our results for the case of zero temperature as well as for the case of non-zero temperature.
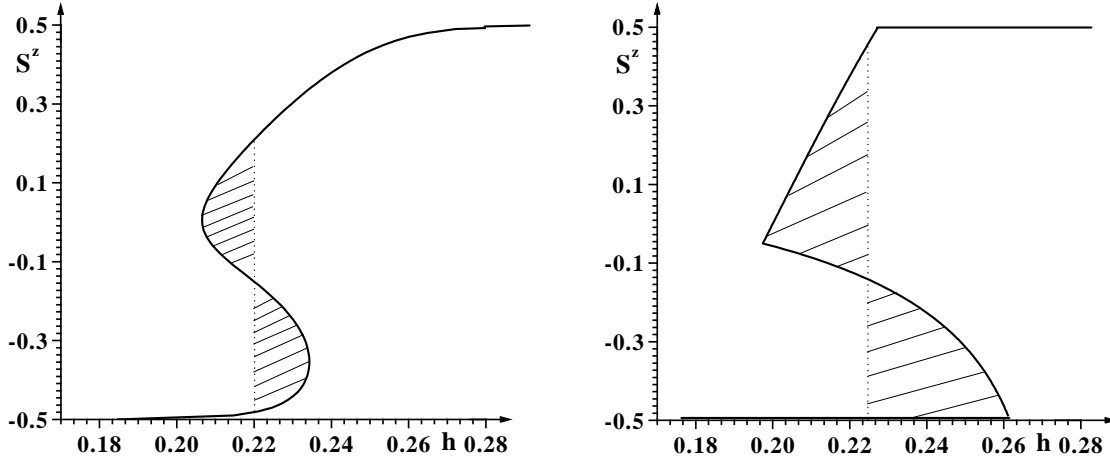

Figure 2. Phase diagram μ - h. Dotted and thin solid lines surround regions with $S^z = \pm\frac{1}{2}$, respectively. Thick solid line indicate the first order phase transition points. a) the case of zero temperature; b) $T = 0.002$ ($W = 0.2$; $g = 1$).

The phase diagrams μ-h which indicate stability regions for states with $\langle S^z\rangle = \pm\frac{1}{2}$ are shown in figure 2 for $g \gg W$.

One can see two regions of the μ and h values where the states with $\langle S^z\rangle = \frac{1}{2}$ and $\langle S^z\rangle = -\frac{1}{2}$ are both stable. In the vicinity of these regions the phase transitions of the first order with the change of the longitudinal field h and/or chemical potential μ take place and they are shown by thick lines on phase diagrams in figure 2.

The field dependencies of $\langle S^z\rangle$ and Ω near the phase transition point are presented in figures 3, 4. Their behaviour in the cases of $T = 0$ and $T \neq 0$ with the change of the chemical potential is similar: S-like for the mean value of the pseudospin and a fish tail form for the thermodynamic potential.
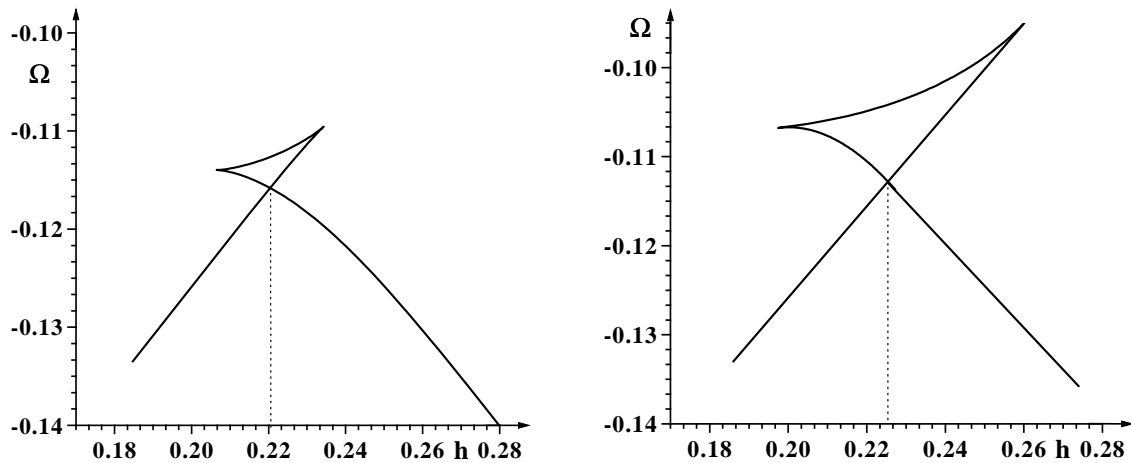
Figure 3. Field dependency of $\langle S^z \rangle$ ($W = 0.2$, $\mu = -0.4$, $g = 1.0$) for μ=const regime; $T = 0.01$ and $T = 0$.
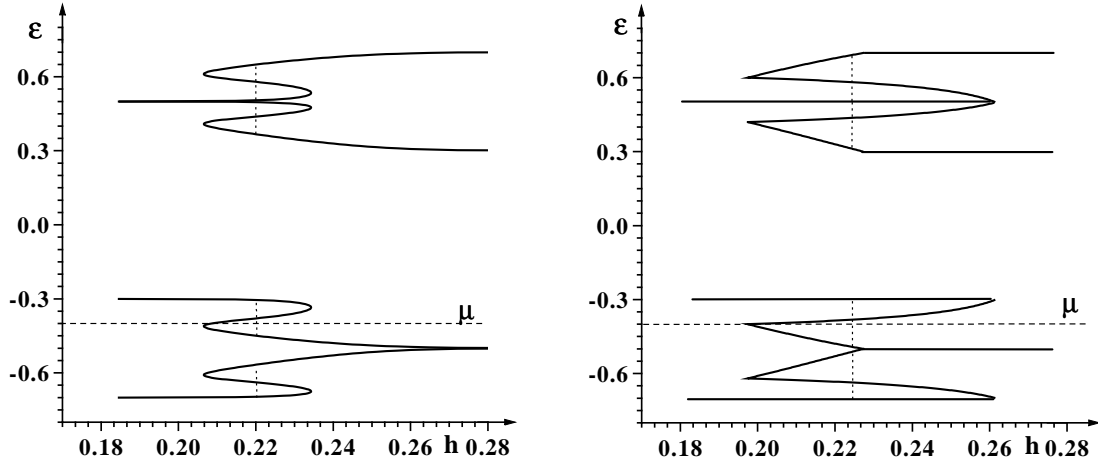
In the μ=const regime, the chemical potential can appear in the electron bands or out of them with the change of field h (dashed line in figure 5), and in the vicinity of the phase transition point this results in a rapid change of electron concentration (dotted lines in figure 6) due to a charge transfer from/to the reservoir (CuO planes). The widths of the electron subbands depend on the mean value of the pseudospin which results in the presented above behaviours.

The phase transition point is presented by a crossing point on the dependence $\Omega(h)$ (figure 4). At the same time this value is determined according to the Maxwell rule from the plot of function $S^z(h)$.
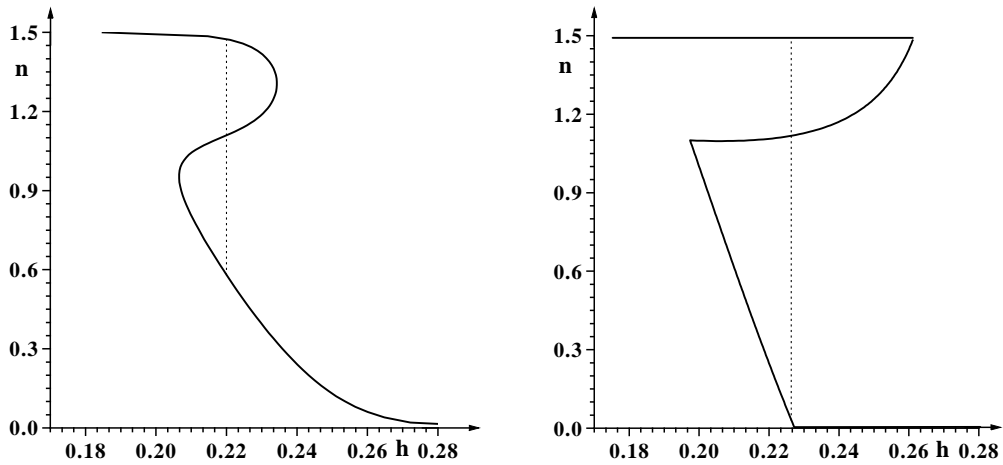

Figure 4. Field dependency of thermodynamic potential ($W = 0.2$, $\mu = -0.4$, $g = 1.0$); $T = 0.01$ and $T = 0$.

With the temperature increase the region of phase coexistence narrows, and the corresponding phase diagram T_c-h is shown in figure 7a. The tilt of the coexistence

Figure 5. Field dependency of electron bands boundaries ($W = 0.2$, $\mu = -0.4$, $g = 1.0$); $T = 0.01$ and $T = 0$.
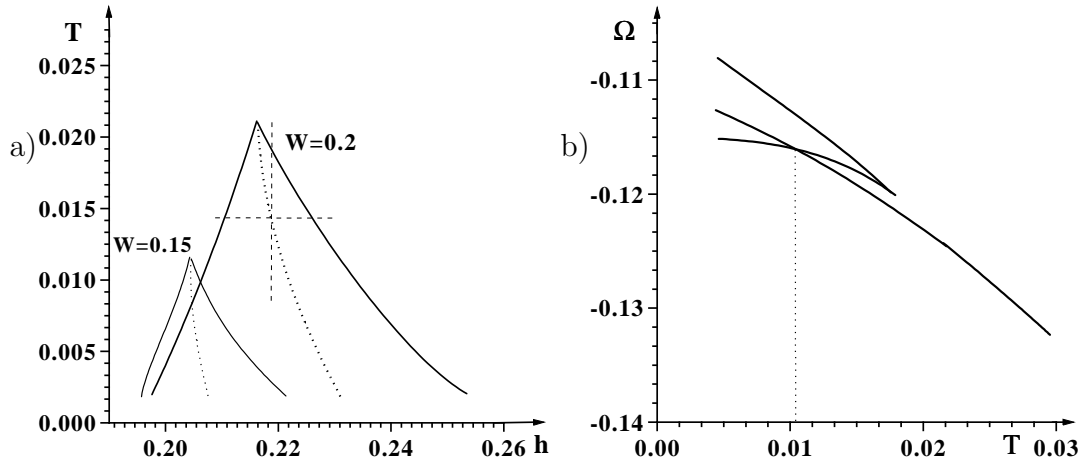

Figure 6. Field dependency of electron concentration ($W = 0.2$, $\mu = -0.4$, $g = 1.0$); $T = 0.01$ and $T = 0$.

curve testifies to the possibility of the first order phase transition at a change of temperature with a jump of the pseudospin mean value. (The phase diagram T_c-μ has a similar form). The existence of the shifted and tilted coexistence curve as the result of the local pseudospin-electron interaction was obtained for the first time in [12] for a pseudospin-electron model with a direct interaction between pseudospins.

The analysis of the thermodynamic potential behaviour with the temperature increase (figure 7b) shows that the lowest value of $\Omega(T)$ corresponds to the jump of the mean value of the pseudospin (dotted lines in figure 8) from the branch which corresponds to the low temperature phase to that of the hight temperature phase. The analysis of the $\langle S^z S^z \rangle$ behaviour with the temperature decrease shows that the high temperature phase is stable up to zero temperature. This means that the vertical line on the T_c-h phase diagram only once crosses the boundary of the phase stability.

In figures the case when the chemical potential is placed in the lower subband is presented. There is no specific behaviour when the chemical potential is placed out of the bands. And if the chemical potential is placed in the upper subband our results transform according to the internal symmetry of the Hamiltonian:

$$\mu \to -\mu, \qquad h \to 2g - h, \qquad n \to 2 - n, \qquad S^z \to -S^z. \qquad (7.1)$$

Figure 7. a) phase diagram T_c-h ($g = 1$, $\mu = -0.4$); b) temperature dependence of the thermodynamic potential ($W = 0.2$, $h = 0.22$, $\mu = -0.4$, $g = 1$).

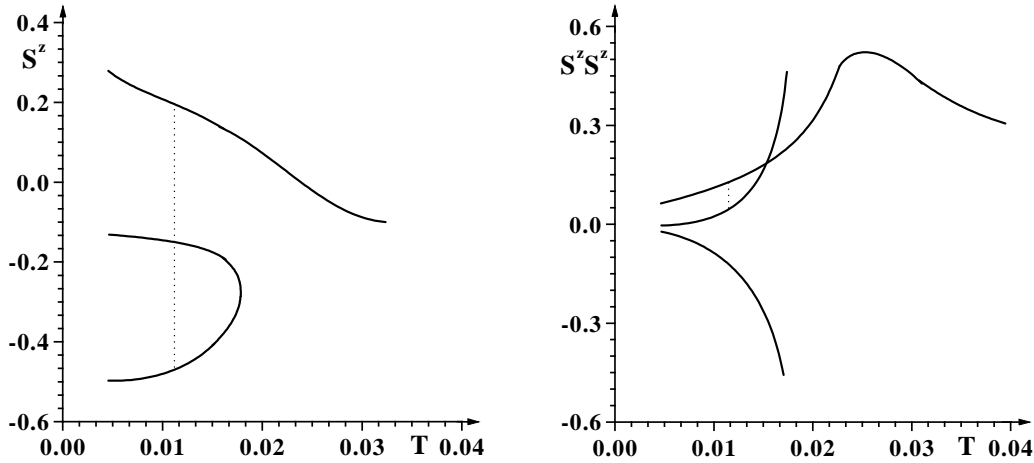## 8. Numerical research in the $n = \text{const}$ regime

In the regime of a fixed value of electron concentration the first order phase transition with a jump of the pseudospin mean value accompanied by a change of electron concentration transforms into a phase separation.

The dependence of the mean value of the particle number (or electron concentration) on the chemical potential is one of the factors determining thermodynamically

stable states of the system. One can see the regions with $\mathrm{d}\mu/\mathrm{d}n \leqslant 0$ where states with a homogenous distribution of particles are unstable, which corresponds to the phase separation into the regions with different electron concentrations and pseudospin mean values (figures 9 and 10).

In the n=const regime the equilibrium condition is determined by the minimum of free energy $F = \Omega + \mu N$. In the phase separated region the free energy as a function of n deflects up (figure 10) and concentrations of the separated phases are determined by the tangent line touch points (these points are also the points of binodal lines which are determined according to the Maxwell rule from the function $\mu(n)$, see figure 9).

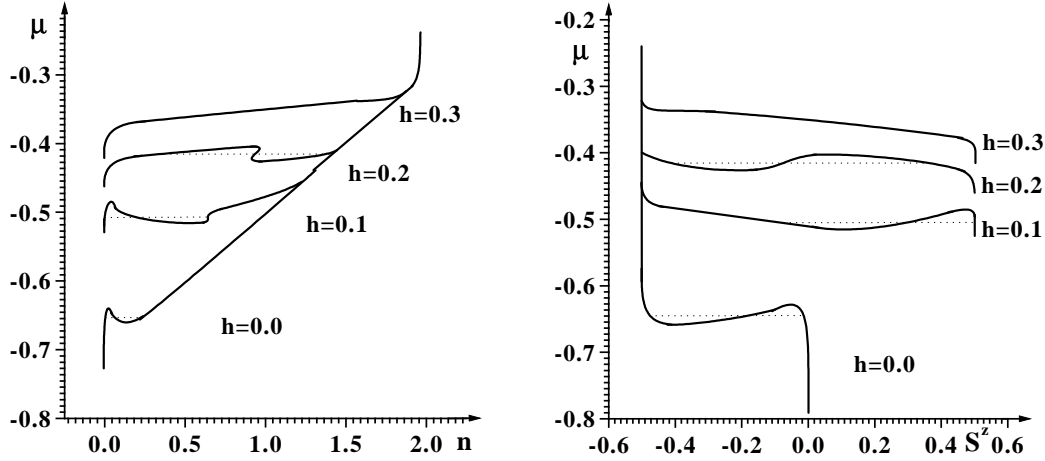The resulting phase diagram T-n is shown in figure 11.

Figure 8. Dependence of the mean value of the pseudospin and the pseudospin-pseudospin correlation function on temperature ($W = 0.2$, $h = 0.22$, $\mu = -0.4$, $g = 1$).
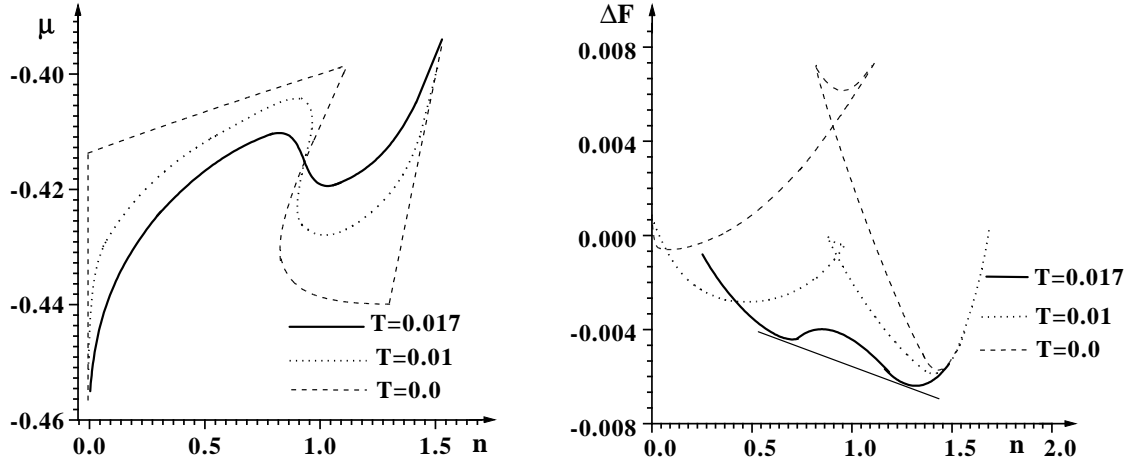
9. Conclusions

Investigation of a pseudospin-electron model in the case of electron correlation absence was performed in the mean field approximation using the Hubbard-I approximation for the calculation of a single-particle Green function. We presented the analytical consideration of our model and all the quantities were obtained within the framework of one self-consistent approximation.

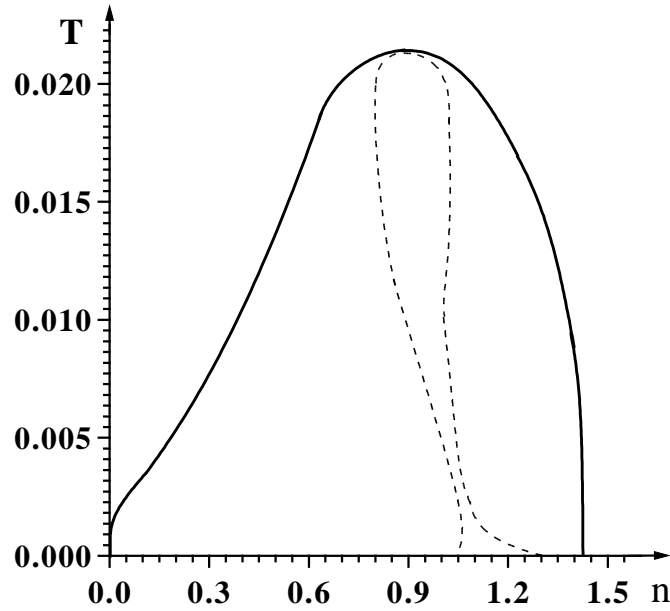As the result of numerical investigations we have obtained:

1) there is always a gap in the electron spectrum (with a change of the mean value of the pseudospin a reconstruction of the electron spectrum takes place);

2) the possibility of the first order phase transition with a change of the longitudinal field h (as a consequence of this the S-like behaviour of the mean value of the pseudospin with a jump in the phase transition point (which corresponds to the inflected point on the dependence $\Omega(h)$) is obtained and at this point the concen-

Figure 9. Dependence of the chemical potential μ on the electron concentration n and the pseudospin mean value $\langle S^z \rangle$ for different h values ($g = 1$, $W = 0.2$, $T = 0.01$).

Figure 10. Dependence of the chemical potential μ on the electron concentration n and deviation of the free energy from linear dependence for different T values ($g = 1$, $W = 0.2$, $h = 0.2$).

Figure 11. Phase diagram T-n ($g = 1$, $W = 0.2$ $h = 0.2$) for a phase separated state. Solid line indicates binodal points, dashed line indicates spinodal points.

tration rapidly redistributes between the conducting sheets CuO_2 and the charge reservoir (CuO planes) in YBaCuO-type structures);

3) the phase coexistence curve is tilted from the vertical line, therefore, there exists a possibility of the first order phase transition with the temperature change;

4) the high temperature phase is stable in the whole region of temperatures (figure 8);

5) in the regime n=const we have the regions with $d\mu/dn < 0$, which corresponds to phase separation with the appearance of regions with different electron concentrations and different orientations of pseudospins.

Analytical expressions for the mean values, thermodynamic functions and susceptibilities of such a simplified pseudospin-electron model ($U = 0$, $\Omega = 0$) were obtained for the uniform phase, when $\langle S_i^z \rangle = \langle S^z \rangle$, and only the possibilities of phase transitions with uniform changes ($\boldsymbol{q} = 0$) were analysed numerically. On the other hand, it is known that for certain parameter values the charge ordered phase can exist in a strong coupling limit of the pseudospin-electron model ($U \to \infty$) [13] which calls for the consideration of the possible superstructure orderings in the opposite limit of $U = 0$ and will be the subject of our further investigations.

References

1. Cohen R.E., Pickett W.E., Krakauer H. Theoretical determination of strong electron-phonon coupling in $YBa_2Cu_3O_7$. // Phys. Rev. Lett., 1990, vol. 64, No. 21, p. 2575–2578.

2. Maruyama H., Ishii T., Bamba N., Maeda H., Koizumi A., Yoshikawa Y., Yamazaki H. Temperature dependence of the EXAFS spectrum in $YBa_2Cu_3O_{7-\delta}$ compounds. // Physica C, 1989, vol. 160, No. 5/6, p. 524.

3. Conradson S.D., Raistrick I.D. The axial oxygen atom and superconductivity in $YBa_2Cu_3O_7$. // Science, 1989, vol. 243, No. 4896, p. 1340.

4. Müller K.A. // Phase transition, 1988, (Special issue).

5. Bishop A.R., Martin R.L., Müller K.A., Tesanovic Z. Superconductivity in oxides: Toward a unified picture. // Z. Phys. B - Condensed Matter, 1989, vol. 76, No. 1, p. 17–24.

6. Hirsch J.E., Tang S. Effective interactions in an oxygen-hole metal. // Phys. Rev. B, 1989, vol. 40, No. 4, p. 2179–2186.

7. Frick M., von der Linden W., Morgenstern I., Raedt H. Local anharmonic vibrations, strong correlations and superconductivity: A quantum simulation study. // Z. Phys. B - Condensed Matter, 1990, vol. 81, No. 2, p. 327–335.

8. Stasyuk I.V., Shvaika A.M. Dielectric properties and electron spectrum of the Müller model in the HTSC theory. // Acta Physica Polonica A, 1993, vol. 84, No. 2, p. 293–313.

9. Izyumov Yu.A., Letfulov B.M. Spin fluctuations and superconducting states in the Hubbard model with a strong Coulomb repulsion. // J. Phys. - Condens. Matter, 1991, No. 3, p. 5373.

10. Izyumov Yu.A., Letfulov B.M. Diagram technique for Hubbard operators. Phase diagram for $(t - J)$-model. Preprint USSR Acad. Sci. Ural Div., 90/2, 1990, 72 p.

11. Stasyuk I.V., Shvaika A.M. Dielectric instability and local anharmonic model in the theory of high-T_c superconductivity. // Physica C, 1994, vol. 235–240, p. 2173–2174.

12. Stasyuk I.V., Havrylyuk Yu. Phase transitions in pseudospin-electron model with direct interaction between pseudospins. Preprint of the Institute for Condensed Matter Physics, ICMP-98-18E, Lviv, 1998, 20 p.

13. Stasyuk I.V., Shvaika A.M. Dielectric instability and vibronic-type spectrum of local anharmonic model of high-T_c superconductors. // Ferroelectrics, 1997, vol. 192, p. 1–10.

14. Stasyuk I.V., Shvaika A.M. Pseudospin-electron model in large dimensions. Preprint of the Institute for Condensed Matter Physics, ICMP–98–20E, Lviv, 1998, 16 p.

15. Stasyuk I.V., Trachenko K.O. Investigation of locally anharmonic models of structural phase transitions. Seminumerical approach. // Cond. Matt. Phys., 1997, No. 9, p. 89–107.

16. Danyliv O.D. Phase transitions in the two-sublattice pseudospin-electron model of high temperature superconducting systems. // Physica C, 1998, vol. 309, p. 303–314.

17. Gervais F. Oxygen polarizability in ferroelectrics. A clue to understanding superconductivity in oxides? // Ferroelectrics, 1992, vol. 130, p. 45–76.

18. Kurtz S.K., Hardy J.R., Floken J.W. Structural phase transition, ferroelectricity and high-temperature superconductivity. // Ferroelectrics, 1988, vol. 87, p. 29–40.

Tabunshchyk K.V. e-mail: tkir@icmp.lviv.ua